Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Computational Prediction of Au(I)-Pb(II) Bonding in Coordination Complexes and Study of the Factors Affecting to the Formation of Au(I)-E(II) (E = Ge, Sn, Pb) Covalent Bonds.

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ELECTRONIC SUPPLEMENTARY INFORMATION

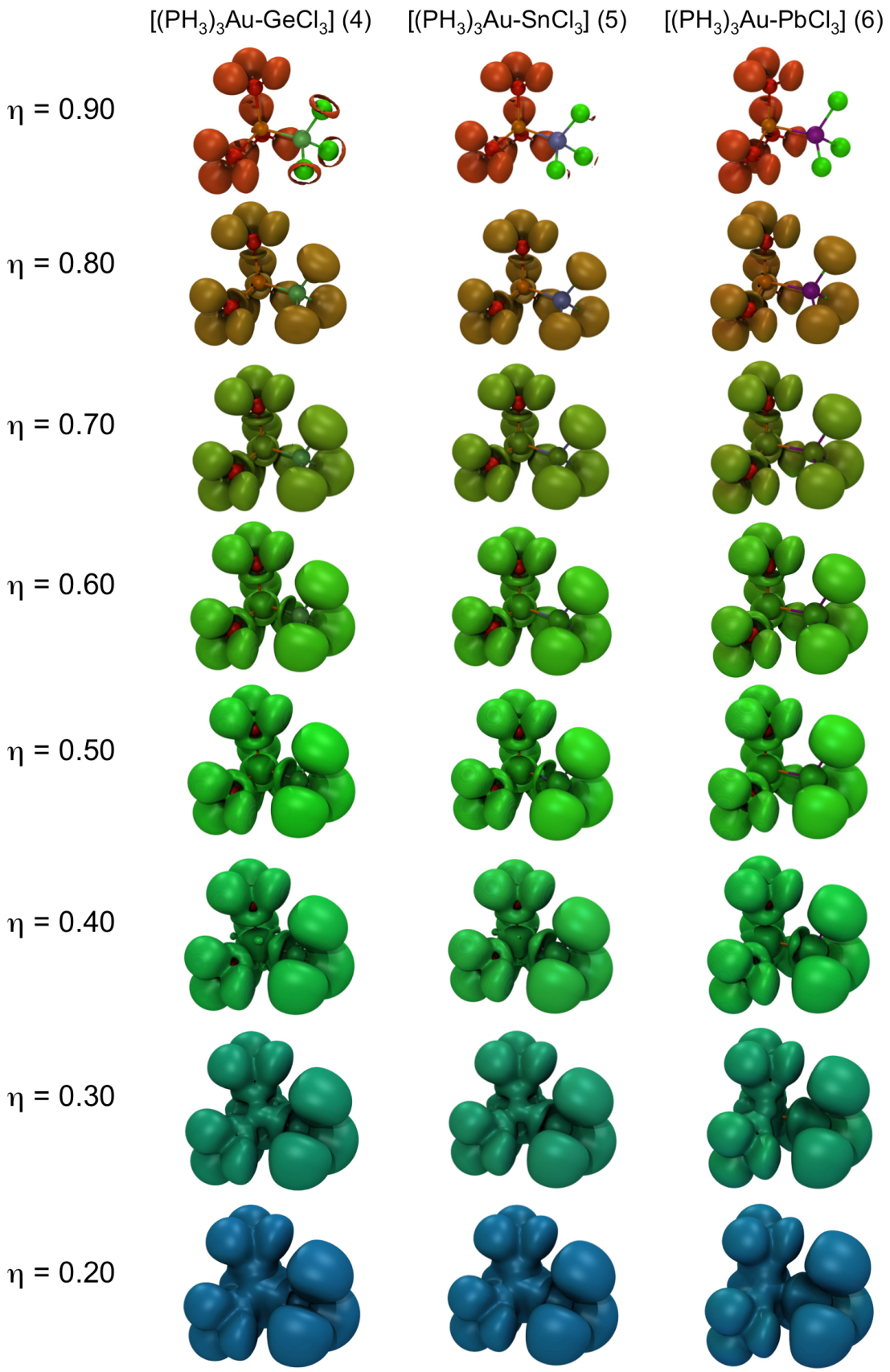

Figure S1. ELF *f*-localization domains for model systems **4**-**6**. For a defined value of *f*, the *f* -localization domain bears all points where ELF takes values larger than *f* ($\eta > f$). They can be visualized by isosurfaces with $\eta = f$.

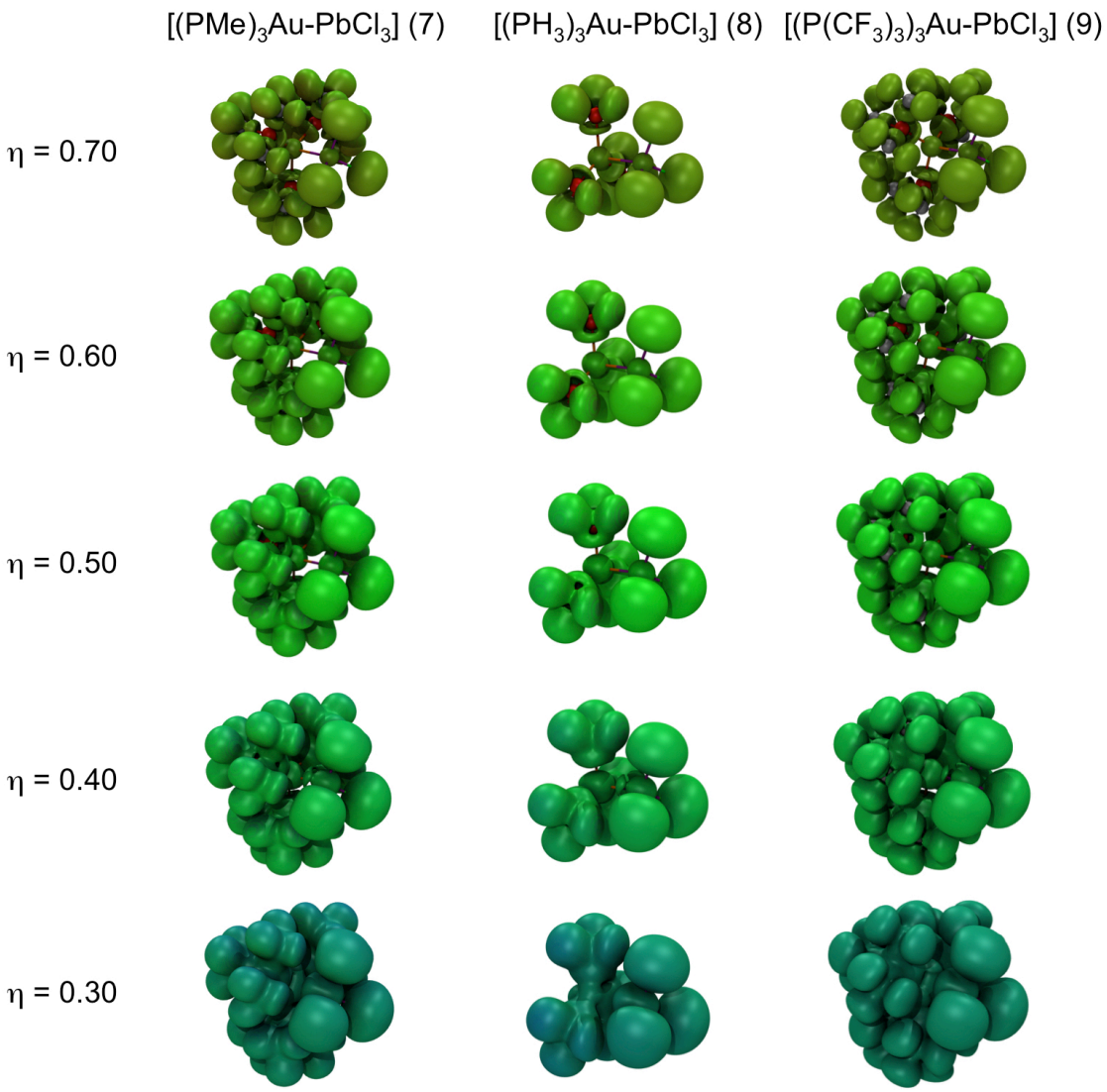

Figure S2. ELF *f*-localization domains for model systems **7**-**9**. For a defined value of *f*, the *f* -localization domain bears all points where ELF takes values larger than *f* (η > *f*). They can be visualized by isosurfaces with η = *f*.

XYZ COORDINATES FOR MODEL SYSTEMS 1-9

Model 1

Ge	-0.00000000	0.00000000	0.69864204
Cl	-1.71567681	-0.99054647	-0.43845346
Cl	0.00000000	1.98109293	-0.43845346
Cl	1.71567681	-0.99054647	-0.43845346

Model 2

Sn	0.00000000	0.00000000	0.62521691
Cl	0.94149020	1.89432598	-0.61271229
Cl	1.16978932	-1.76251742	-0.61271229
Cl	-2.11127952	-0.13180855	-0.61271229

Model 3

Pb	-0.00000000	-0.00000000	-0.46144174
Cl	-1.94888918	-1.12519169	0.74181362
Cl	1.94888918	-1.12519169	0.74181362
Cl	-0.00000000	2.25038339	0.74181362

Model 4

Au	-0.03502000	-0.99630600	0.00000000
Ge	0.05021000	1.42838900	0.00000000
Cl	1.06576700	2.35211500	1.70170900
Cl	1.06576700	2.35211500	-1.70170900
Cl	-1.87985800	2.45565500	0.00000000
P	-2.30225900	-1.54001300	0.00000000
P	1.06576700	-1.65841200	-1.94573300
P	1.06576700	-1.65841200	1.94573300
H	-2.87255600	-2.26580800	-1.05506700
H	-2.87255600	-2.26580800	1.05506700
H	-3.17920300	-0.44979200	0.00000000
H	1.56003500	-0.61639200	-2.73788800
H	0.39847900	-2.38079300	-2.94476900
H	2.22478200	-2.44500200	-1.88970000
H	1.56003500	-0.61639200	2.73788800
H	0.39847900	-2.38079300	2.94476900
H	2.22478200	-2.44500200	1.88970000

Model 4b

Au	-0.63622752	1.12275447	0.00000000
Ge	-0.63622852	1.12275447	-2.42619200
Cl	0.34647448	2.82433447	-3.38502400
Cl	0.34602848	-0.57908353	-3.38502400
Cl	-2.60119252	1.12301247	-3.38502200
P	1.61051248	1.12245947	0.62301700
P	-1.75933852	3.06863447	0.62302800
P	-1.75984952	-0.82283153	0.62302800
H	2.15509948	2.17745547	1.36839800
H	2.15482248	0.06732147	1.36839800
H	2.52521348	1.12234047	-0.43572600
H	-2.21659352	3.86084947	-0.43571100
H	-1.11770752	4.06758647	1.36840400
H	-2.94527752	3.01275747	1.36841800
H	-2.21731152	-1.61492653	-0.43571100
H	-1.11848052	-1.82195153	1.36840400
H	-2.94577352	-0.76664253	1.36841800

Model 5

Au	-0.02218600	-1.21240000	0.00000000
Sn	0.02514400	1.37413700	0.00000000
Cl	1.09903000	2.40646100	1.82699300
Cl	1.09903000	2.40646100	-1.82699300
Cl	-2.06489000	2.46436000	0.00000000
P	-2.29509200	-1.72618600	0.00000000
P	1.09903000	-1.78828800	-1.95992400
P	1.09903000	-1.78828800	1.95992400
H	-3.16881100	-0.63381900	0.00000000
H	-2.85999800	-2.45266300	-1.05671800
H	-2.85999800	-2.45266300	1.05671800
H	1.56541800	-0.72044000	-2.73376800
H	0.44628000	-2.51316000	-2.96591600
H	2.27626300	-2.54663700	-1.90919900
H	1.56541800	-0.72044000	2.73376800
H	0.44628000	-2.51316000	2.96591600
H	2.27626300	-2.54663700	1.90919900

Model 5b

Au	1.30988019	0.79341316	0.00000000
Sn	3.89685019	0.79341416	-0.00163700
Cl	4.94749219	1.84823416	-1.82929500
Cl	4.94980419	1.84823416	1.82469100
Cl	4.94865219	-1.31621584	-0.00230200
P	0.75459619	3.05653916	0.00035100
P	0.75336219	-0.33815084	-1.95957200
P	0.75584219	-0.33815084	1.96027500
H	1.83079519	3.95009716	-0.00032900
H	0.01723719	3.60805916	-1.05590000
H	0.01857419	3.60805916	1.05753500
H	1.82907519	-0.78492384	-2.73409700
H	0.01603319	0.30122816	-2.96509800
H	0.01671119	-1.52906184	-1.90838100
H	1.83253419	-0.78492384	2.73343800
H	0.01978619	0.30122816	2.96673300
H	0.01912719	-1.52906184	1.91001600

Model 6

Au	-0.01235500	-1.52319700	0.00000000
Cl	1.14390600	2.26379600	1.94943100
Cl	1.14390600	2.26379600	-1.94943100
Cl	-2.23249800	2.29118800	0.00000000
P	-2.33069200	-1.74347100	0.00000000
P	1.14390600	-1.77165200	-2.00612500
P	1.14390600	-1.77165200	2.00612500
H	-3.02594300	-0.52872500	0.00000000
H	-2.96621900	-2.39565300	-1.06214400
H	-2.96621900	-2.39565300	1.06214400
H	1.50623800	-0.56548500	-2.61674400
H	0.53386000	-2.42404400	-3.08297900
H	2.37348700	-2.43896000	-2.02083400
H	1.50623800	-0.56548500	2.61674400
H	0.53386000	-2.42404400	3.08297900
H	2.37348700	-2.43896000	2.02083400
Pb	0.00988000	1.21819400	0.00000000

Model 6b

Au	0.06736527	0.50893841	0.00666237
Cl	-0.88489473	4.47480241	1.99536637
Cl	-0.88489473	4.47480241	-1.98204163
Cl	-3.87244173	2.75895741	0.00666237
P	2.20601627	1.55564241	0.00666237
P	-0.88489473	-0.21923459	2.06403937
P	-0.88489473	-0.21923459	-2.05071463
H	2.13722427	2.96398541	0.00666237
H	3.10422727	1.35699341	1.07344937
H	3.10422727	1.35699341	-1.06012463
H	-1.78708373	0.71028141	2.62100937
H	-0.07014573	-0.46795059	3.18592337
H	-1.67397873	-1.38485259	2.11860137
H	-1.78708373	0.71028141	-2.60768463
H	-0.07014573	-0.46795059	-3.17259863
H	-1.67397873	-1.38485259	-2.10527663
Pb	-1.36957973	3.01264841	0.00666237

Model 7

Au	0.00000	0.00000	-1.33053
P	-2.06329	-1.19124	-1.35495
P	2.06329	-1.19124	-1.35495
P	0.00000	2.38249	-1.35495
Pb	0.00000	0.00000	1.66842
Cl	2.00482	1.15748	2.73809
Cl	0.00000	-2.31496	2.73809
Cl	-2.00482	1.15748	2.73809
C	0.00000	3.14512	-3.00803
H	0.00000	4.23461	-2.93307
H	0.88352	2.82344	-3.55962
H	-0.88352	2.82344	-3.55962
C	2.72375	-1.57256	-3.00803
H	2.88693	-0.64657	-3.55962
H	3.66728	-2.11730	-2.93307
H	2.00341	-2.17687	-3.55962
C	-2.72375	-1.57256	-3.00803
H	-3.66728	-2.11730	-2.93307
H	-2.88693	-0.64657	-3.55962
H	-2.00341	-2.17687	-3.55962
C	1.42247	3.16158	-0.53853
H	1.31874	4.24874	-0.53041
H	1.51200	2.79796	0.48777
H	2.33494	2.89086	-1.07058
C	-1.42247	3.16158	-0.53853
H	-1.51200	2.79796	0.48777
H	-1.31874	4.24874	-0.53041
H	-2.33494	2.89086	-1.07058
C	2.02677	-2.81269	-0.53853
H	3.02014	-3.26643	-0.53041
H	1.66710	-2.70841	0.48777
H	1.33608	-3.46755	-1.07058
C	-2.02677	-2.81269	-0.53853
H	-1.66710	-2.70841	0.48777
H	-3.02014	-3.26643	-0.53041
H	-1.33608	-3.46755	-1.07058
C	-3.44925	-0.34889	-0.53853
H	-4.33889	-0.98230	-0.53041
H	-3.17910	-0.08955	0.48777
H	-3.67103	0.57669	-1.07058
C	3.44925	-0.34889	-0.53853
H	3.17910	-0.08955	0.48777
H	4.33889	-0.98230	-0.53041
H	3.67103	0.57669	-1.07058

Model 8

Au	-0.01589	-1.60837	0.00000
Cl	1.17086	2.29374	1.98870
Cl	1.17086	2.29374	-1.98870
Cl	-2.27420	2.32669	-0.00000
P	-2.39321	-1.74166	-0.00000
P	1.17086	-1.77763	-2.05738
P	1.17086	-1.77763	2.05738
H	-3.02216	-0.47968	-0.00000
H	-3.07944	-2.35431	-1.06679
H	-3.07944	-2.35431	1.06679
H	1.50302	-0.52559	-2.61435
H	0.58192	-2.39312	-3.17926
H	2.42929	-2.40825	-2.11194
H	1.50302	-0.52559	2.61435
H	0.58192	-2.39312	3.17926
H	2.42929	-2.40825	2.11194
Pb	0.01259	1.27825	-0.00000

Model 8b

Au	-0.35179639	1.31736525	0.00000000
Cl	-1.30405639	5.28322925	1.98870400
Cl	-1.30405639	5.28322925	-1.98870400
Cl	-4.29160339	3.56738425	0.00000000
P	1.78685461	2.36406925	0.00000000
P	-1.30405639	0.58919225	2.05737700
P	-1.30405639	0.58919225	-2.05737700
H	1.71806261	3.77241225	0.00000000
H	2.68506561	2.16542025	1.06678700
H	2.68506561	2.16542025	-1.06678700
H	-2.20624539	1.51870825	2.61434700
H	-0.48930739	0.34047625	3.17926100
H	-2.09314039	-0.57642575	2.11193900
H	-2.20624539	1.51870825	-2.61434700
H	-0.48930739	0.34047625	-3.17926100
H	-2.09314039	-0.57642575	-2.11193900
Pb	-1.78874139	3.82107525	0.00000000

Model 9

Au	0.02532	0.14391	-0.25258
P	2.02509	-0.66165	-1.24988
P	0.17883	2.39281	0.50929
P	-2.00930	-0.34007	-1.38430
Pb	-0.18913	-1.36871	2.07838
C	3.01983	0.57723	-2.29203
C	0.48751	3.75691	-0.77990
C	-2.47664	0.84114	-2.79660
Cl	-0.23777	-3.78387	1.61356
Cl	-2.16830	-1.07001	3.49717
Cl	1.62708	-1.19939	3.72072
C	-1.33087	3.10792	1.41574
C	1.55253	2.77712	1.76600
C	3.37767	-1.31853	-0.08267
C	1.88942	-2.10170	-2.48134
C	-3.59905	-0.31021	-0.33814
C	-2.22073	-2.02025	-2.24848
F	1.37706	-1.62561	-3.61589
F	-1.48039	-2.01398	-3.35613
F	3.54201	-0.45815	0.90712
F	2.68085	2.21762	1.34903
F	-2.27588	3.35250	0.50879
F	-3.54535	0.71586	0.49751
F	-4.69272	-0.19104	-1.07913
F	-3.66369	-1.43681	0.35103
F	-1.06371	4.23275	2.06115
F	-1.77744	2.21583	2.28018
F	1.76110	4.07811	1.91475
F	1.21054	2.25674	2.93252
F	4.54149	-1.48395	-0.69761
F	2.97448	-2.48158	0.40231
F	3.05108	-2.67442	-2.75055
F	1.06969	-3.01447	-1.98699
F	-3.47756	-2.26956	-2.58413
F	-1.79476	-2.97634	-1.44549
F	-3.44705	0.39608	-3.57719
F	-1.39687	1.04857	-3.54477
F	-2.85370	2.00039	-2.26237
F	-0.27275	3.51370	-1.84292
F	1.76402	3.70347	-1.15014
F	0.22115	4.97746	-0.34499
F	3.63492	1.42292	-1.47069
F	3.92309	0.01274	-3.07671
F	2.17196	1.26419	-3.05316